Computational indentation in highly cross-linked polymer networks

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Abstract

Indentation is a common experimental technique to study the mechanics of polymeric materials. The main advantage of using indentation is this provides a direct correlation between the microstructure and the small-scale mechanical response, which is otherwise difficult within the standard tensile testing. The majority of studies have investigated hydrogels, microgels, elastomers, and even soft biomaterials. However, a less investigated system is the indentation in highly cross-linked polymer (HCP) networks, where the complex network structure plays a key role in dictating their physical properties. In this work, we investigate the structure-property relationship in HCP networks using the computational indentation of a generic model. We establish a correlation between the local bond breaking, network rearrangement, and small-scale mechanics. The results are compared with the elastic-plastic deformation model. HCPs harden upon indentation.

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